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LETTER TO THE EDITOR

Local separatrices for Hamiltonians with symmetries

L Wiesenfeld

Laboratoire de Spectrométrie Physique, Université Joseph-Fourier-Grenoble, F-38402 Saint-Martin-d'Hères-Cedex, France
and
Laboratoire d'Astrophysique de l'Observatoire de Grenoble, Université Joseph-Fourier-Grenoble, F-38051, Grenoble Cedex 9, France

E-mail: laurent.wiesenfeld@ujf-grenoble.fr

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Abstract
We consider dynamics generated by Hamiltonians with three degrees of freedom and symmetries. It is shown that locally, away from a possible saddle equilibrium, some codimension-1 invariant manifold may exist. They are stable/unstable manifolds of a codimension-2 hyperbolic invariant manifold. This structure appears when some periodic orbits constitutive of the Arnold web have bifurcated and become linearly unstable. This result generalizes the existence of normally hyperbolic invariant manifolds and their codimension-1 stable/unstable manifolds in the vicinity of an unstable $\otimes$ (stable)^2 equilibrium point.

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1. Introduction

Manifolds that are invariant under the flow are of special importance for the study of phase space structure associated with a Hamiltonian H. Among the various possible invariant manifolds, some are of special interest: those having a codimension 1 (codim 1) in the full phase space or in the energy level. They are the largest invariant structures possible and as such, they determine to some extent transport in phase space [1]. They also constitute, at least locally, separatrices in phase space which are generalizations of the usual separatrices of unstable equilibrium points in one degree of freedom (1-DOF) Hamiltonians. For $n > 2$ DOF Hamiltonian dynamics, the overall geometry of invariant objects in phase space is vastly more complicated and less known than for 2-DOF Hamiltonians. Although several specific n-DOF codim-1 invariant manifolds have been known for a long time, there has recently been a renewed interest in those invariant manifolds associated with *transition states*.

The geometry of phase space has been elucidated in the neighbourhood of a certain class of equilibrium points P: $\nabla H(P) = 0$, with linear stability of the type saddle $\otimes$ (centre)$^{n-1}$

[2, 3]. These equilibrium points generate centre and stable/unstable manifolds resulting in a general yet algorithmic construction of normally hyperbolic invariant manifolds (NHIM) and transition states, that extend into the non-linear regime. NHIMs are codim 2 in phase space, while stable and unstable manifolds of NHIMs are codim 1. They act as impenetrable barriers in phase space. Also, NHIMs and their stable/unstable manifolds are the support of transition states that act as gates connecting disjoint regions of phase space. The importance of those multi-dimensional phase space transition states has been underlined and recently used in many areas of physics and astronomy [4–7].

As stated, the NHIM and the associated transition states (TS) structures have been proved to exist only in the vicinity of saddle $\otimes$ (centre)$^{n-1}$ equilibrium points. No general analogous result exists in the neighbourhood of a (centre)^n equilibrium point, in the vicinity of which Arnold web structure is supposed to exist [8, 9].

In this letter, I wish to show that under certain restrictive conditions at least, other large invariant unstable structures exist. These hyperbolic invariant manifolds are codim 2 and have in analogy with NHIMs stable and unstable manifolds, of codim 1. Whether or not these structures support transition seems to depend on some stability analysis that will be presented.

2. Separatrices and invariant manifolds

To begin with, let us recall what the situation is for 2-DOF Hamiltonian, which was elucidated some time ago [10, 11]. At an energy superior to that of a stable $\otimes$ unstable equilibrium point P, there exists a periodic orbit named PODS (for periodic orbit dividing surface) which is unstable. The linearized Hamiltonian in the neighbourhood of such an orbit may be written as [12]

$$2H = 2\omega I + p^2 - \kappa^2 q^2 \tag{1}$$

with κ^2 real and I, the action of the periodic orbit, period $2\pi/\omega$ and p, q coordinates normal to it. Let us emphasize that this linearized Hamiltonian is the same as the linearized Hamiltonian proposed for NHIMs [2] and that the PODS is *direct* hyperbolic necessarily. That is, the eigenvalues of the monodromy matrix of the PODS are real and positive. However, it was shown that other types of PODS may also exist, which are not in the vicinity of stable $\otimes$ unstable equilibrium points. These PODS may be either *direct* or *inverse* hyperbolic, with either real positive or real negative eigenvalues of the monodromy matrix. There seems to exist no closed real form of inverse hyperbolic quadratic Hamiltonian, but it could be written as equation (1), with κ^2 complex. Let us recall that in the neighbourhood of a T-periodic inverse hyperbolic periodic orbit, motion is $2T$-periodic, with a winding number of 1 (Möbius strip topology) [12–14].

In the chemical literature, direct hyperbolic PODS have been named ‘repulsive PODS’, while inverse hyperbolic PODS have been named ‘attractive PODS’. They organize phase space in a fairly different way, that was described in detail in [15, 16].

It is very tempting to try to extend these ideas to $n > 2$ degree of freedom Hamiltonians. As stated in the beginning of this letter, this had been possible in the vicinity of some equilibrium points P. Let us assume that $H(P) = E = 0$ (resetting the origin of energy). Then for $0 < E < \overline{E}$, the closure of the Lyapunov stable periodic orbits ($n-2$ times stable, once unstable) constitutes the centre manifold $\mathcal{W}^C(P)$ of P [2, 17, 18]. At each energy level E, the NHIM is defined as

$$\text{NHIM:} \quad \mathcal{W}^C(P) \cap (H = E) \qquad 0 < E < \overline{E}. \tag{2}$$

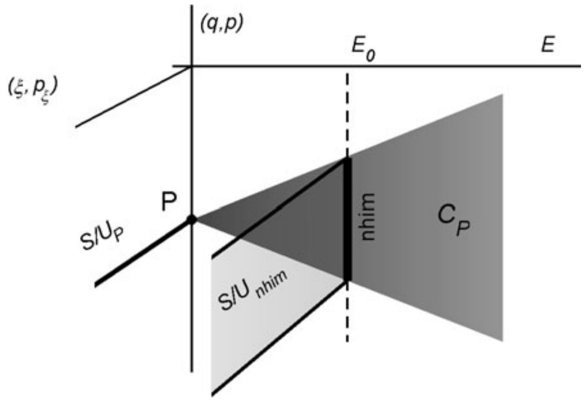

Figure 1. General scheme of the linearized dynamics. (q, p) denotes collectively the bath coordinates and momenta, (p_ξ, ξ), the reaction coordinate and momentum. P is the equilibrium point. C, U, S are respectively centre, unstable, stable manifolds of the object indicated in their respective indices.

The dimension of $\mathcal{W}^C(P)$ is $D(\mathcal{W}^C) = 2n - 2$; the NHIM has thus $D = 2n - 3$ and its stable and unstable manifolds are codim 1, as stated. In a nutshell, the situation is depicted in figure 1.

Let us write down, for $n = 3$ degrees of freedom, the linearized Hamiltonian that supports this whole structure [2, 17]. From this formula, it will be easier to understand where it may be possible to extend those ideas, and where not. Let $H = H(p_i, q_i)$ be the 3-DOF Hamiltonian and the equilibrium point P be at coordinates $p_i = q_i = 0$, $i = 1, \ldots, 3$ with $H(p_i = 0, q_i = 0) = 0$. We linearize H in the vicinity of P and get

$$2H = p_1^2 + \omega_1^2 q_1^2 + p_2^2 + \omega_2^2 q_2^2 + p_\xi^2 - \kappa^2 \xi^2 \tag{3}$$

with $\omega_1, \omega_2, \kappa \in \mathbb{R}^*$ and $\xi, p_\xi \equiv q_3, p_3$. In the chemical literature, ξ is termed the *reaction coordinate*. It is possible to define with help of equation (3) the NHIM as

$$p_\xi = \xi = 0 \tag{4}$$

$$2E = 2H = p_1^2 + \omega_1^2 q_1^2 + p_2^2 + \omega_2^2 q_2^2 \tag{5}$$

$$\omega_1 I_1 + \omega_2 I_2 = E \qquad 0 \leqslant \omega_1 I_1 \quad \omega_2 I_2 \leqslant E. \tag{6}$$

Equation (6) defines the actions $I_{1,2}$ of the two harmonic oscillators. It may also be thought as

$$\omega_1 I_1 = (1 - \mu)E \qquad \omega_2 I_2 = \mu E \qquad 0 \leqslant \mu \leqslant 1. \tag{7}$$

This whole idea may be summarized in the following scheme, figure 2(*a*). It indicates that the structure of the NHIM is in fact an S_3 sphere, foliated by the full family of tori compatible with the energy conservation rule, equation (6). Dimension of this S_3 sphere is 3, leading to stable/unstable manifolds $\mathcal{W}^{u,s}(S_3)$ attached to each point of the sphere by

$$p_\xi = \pm\kappa\xi \qquad H = E. \tag{8}$$

Dimension of $\mathcal{W}^{u,s}(S_3)$ is 4, codim 1 in the five-dimensional energy level $H = E$.

It is the very fact that (7) is fulfilled for the whole segment $0 \leqslant \mu \leqslant 1$ that leads to the full 3-sphere, hence to codim-1 stable and unstable manifolds acting as separatrices. Now, let us try to see and understand what happens away from a saddle equilibrium point, in a potential well. It is well known that in the vicinity of a stable equilibrium point, the situation is totally different. We have a two-parameter family of T_3 tori that foliate phase space, but no structure

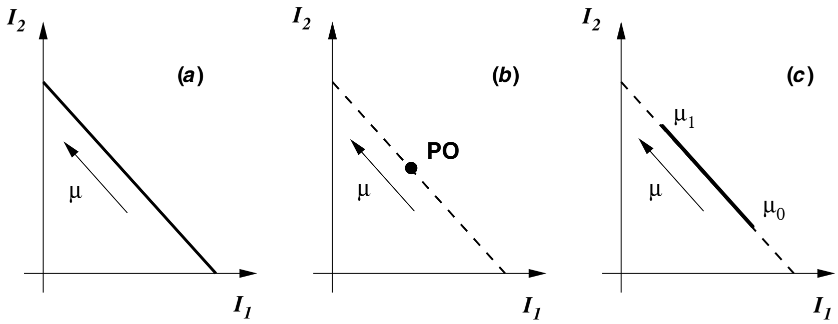

Figure 2. Schemes corresponding to equation (7)—(a), equation (12)—(b) and equation (16)—(c).

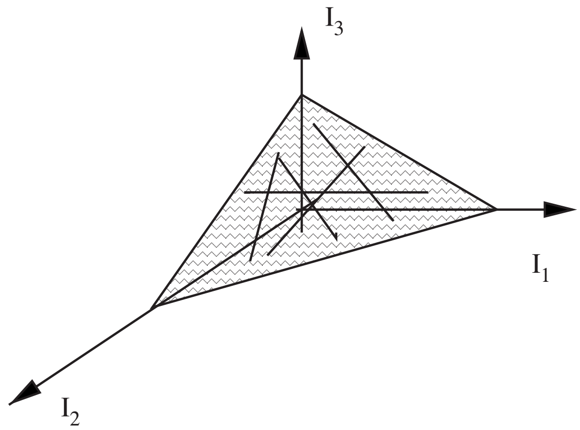

Figure 3. A view of the 3-DOF energy function, when motion is fully stable. The Arnold web is schematized as lines of resonances.

is larger than codim 2:

$$2E = 2H = p_1^2 + \omega_1^2 q_1^2 + p_2^2 + \omega_2^2 q_2^2 + p_3^2 + \omega_3^2 q_2^3 \tag{9}$$

$$\omega_1 I_1 + \omega_2 I_2 + \omega_3 I_3 = E. \tag{10}$$

Equation (6) defines a plane in the three-dimensional space of actions; on that plane resonances may occur, as well as Arnold diffusion, see figure 3.

Let us imagine now that one of the periodic orbits (POs) that constitute the tori undergoes a bifurcation at some energy E^* and becomes unstable beyond, for $E > E^*$. Then the Hamiltonian linearized in the vicinity of that PO reads [12, 18, 19]

$$2E = 2H = I_1 + p_2^2 + \omega_2^2 q_2^2 + p_3^2 - \kappa^2 q_3^2. \tag{11}$$

Here, I_1 is the action associated with the PO, p_2, q_2 are coordinates associated with the modulus 1 eigenvalues of the monodromy matrix of the PO and p_3, q_3 are associated with eigenvalues modulus different from 1 (direct hyperbolic or inverse hyperbolic eigenvalues). We have the structure of what is called in the literature a 'whiskered torus' T_W [1]. The stable and unstable manifolds $p_3 = \pm\kappa q_3$ are codim-2 in the energy level and do not act as separatrices, as is well known. We may think of the whiskered torus as

$$I_1 = (1-\mu)E \qquad I_2 = \mu E \qquad \mu = \mu_{\mathrm{PO}} \tag{12}$$

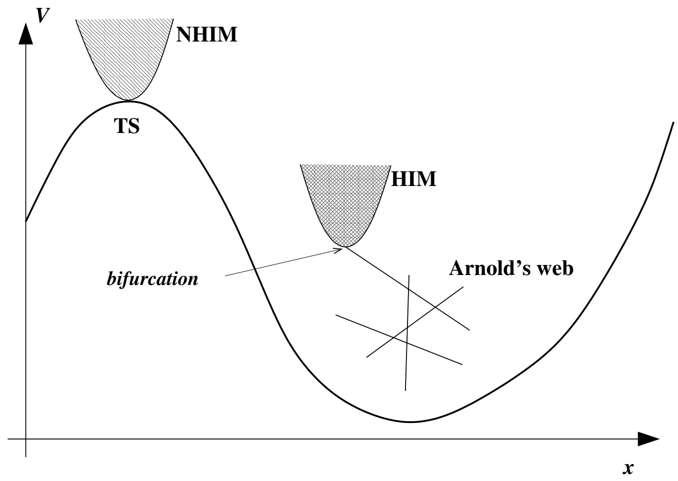

Figure 4. A view of the quasi-regular region at the transition state (TS) [4] and the new HIM in the potential well. x is some collective coordinate, V some potential-like function.

with the sole but crucial difference that the whole S_3 sphere, described by parameter μ is reduced to a single torus, at $\mu = \mu_{\mathrm{PO}}$, figure 2(*b*).

3. Symmetries: new hyperbolic invariant manifolds

To summarize, in order to devise again large invariant manifolds, we have to find a way to recover a whole part of the S_3 sphere. In order to have parts of this sphere and codim-1 stable and unstable manifold, it is necessary to recover—at least partly—equations (6)–(7). While this does not seem possible in generic circumstances, it is possible to recover parts of the S_3 sphere in cases of additional symmetries. Without symmetry, at a given energy, only isolated particular actions give rise to periodic motion, hence isolated whiskered torus. If there is a continuous, one-parameter family of symmetry—let μ be this parameter—then we may recover the situation of a hyperbolic invariant manifold of codim 2.

Let us consider the following type of 3-DOF polynomial Hamiltonian:

$$H = \frac{1}{2} \sum_{i=1,2,3} \left(p_i^2 + \omega_i^2 q_i^2\right) + V_{\mathrm{c}1}(q_1; q_2, q_3) + V_{\mathrm{c}2}(q_2, q_3). \tag{13}$$

We suppose the following properties for H:

(i) Symmetries : $q_1 \leftrightarrow -q_1$, $q_3 \leftrightarrow -q_3$, but $q_2 \leftrightarrow -q_2$ need not be true.
(ii) Couplings are such that $V_{\mathrm{c}1}(q_1; q_2, q_3) = 0$ if $q_1 = 0$ and $V_{\mathrm{c}2}(q_2, q_3) = 0$ if $q_2 = 0$ or $q_3 = 0$.
(iii) The two preceding points entail that $\Gamma_1 \doteq q_1 = p_1 = q_2 = q_2 = 0$ is a periodic orbit, as well as $\Gamma_2 \doteq q_1 = p_1 = q_3 = q_3 = 0$.
(iv) The largest exponent of q_2 in $V_{\mathrm{c}1}$ or $V_{\mathrm{c}2}$ is M. M odd allows for unbound motion.

Point (iii) is the key point: it allows us to recover a parameter μ covering a non-zero segment. Nearby the fully stable equilibrium point $p_i = q_i = 0$, we have the usual structure of tori foliating the phase space, with possible resonances. As soon as one (and one only) of the POs Γ_i undergoes a change of stability, we are in a situation that is similar (but not identical) to equations (5)–(7). Let us write the general linear Hamiltonian describing this situation. One of the periodic orbits Γ_1, Γ_2, say Γ_1, has the following non-trivial eigenvalues of its monodromy matrix [13]: $\lambda_{1,2} = k, 1/k$ with $|k| > 1$, $|\lambda_{3,4}| = 1$, $\lambda_{3,4} = \alpha \pm \mathrm{i}\beta$, with $\alpha \in \mathbb{R}$, $\beta \in \mathbb{R}^*$. Note that $k > 1$ corresponds to a direct hyperbolic stability, $k < -1$ to an inverse hyperbolic stability. The possibility of $k < -1$, analogous to the attractive PODS for 2-DOF systems, is new with respect to transition state type of NHIMs, where $k > 1$ always.

In the vicinity of Γ_1, we may write the linearized Hamiltonian as [18, 19] :

$$2H = \omega_1 I(\Gamma_1; \mu) + h(p_3, q_3; \mu) + p_2^2 - \kappa^2 q_2^2 \tag{14}$$

since the unstable/stable manifolds are contained in the q_2/p_2 hyperplane. For small q_3, we have

$$h(p_3, q_3; \mu) = \omega_2 I(\Gamma_2; \mu) \tag{15}$$

$$\omega_1 I_1 = (1-\mu)E \qquad \omega_2 I_2 = \mu E \qquad 0 \leqslant \mu_0 \leqslant \mu \leqslant \mu_1 \leqslant 1. \tag{16}$$

Contrary to (7), in (16), $\mu_0 \neq 0$ and $\mu_1 \neq 1$, usually. A very schematic view of the new situation is presented in figure 2(*c*) and figure 4.

In principle, equations (13)–(16) complete the argument. The new invariant manifold, let us call it a HIM (for hyperbolic invariant manifold), is defined as $x = p_x = 0$, in a formally completely analogous way to [2] and to (3). As in [2, 17], the HIM has codim 2, and its stable/unstable manifolds, codim 1 in the energy level. However, the interpretation of an HIM is different in two key points from the NHIM of [2, 17]:

(i) Γ_1 or Γ_2 need not be direct hyperbolic. Consequently, even linearized (local) phase space structure nearby the invariant manifold may be different from the structure nearby NHIMs. Γ_1 or Γ_2 need not define transition states.

(ii) What the full consequences of (16) are, where the HIM and its stable/unstable manifolds have borders, is still unclear and justifies more investigations.

4. Conclusion

It may seem that Hamiltonian (13) is quite particular. Let us first keep in mind that (13) is only an expansion of a Hamiltonian nearby a pre-determined periodic orbit. Also, it must be underlined that this type of Hamiltonian is very commonplace in the realm of chemical physics. It could very well be a model that describes the coupling between three vibrational modes with a local to normal transition (bound motion, M even). With M odd—unbound motion possible for $q_2 < 0$—it could describe the dissociation of an excited complex. Under certain circumstances, it may be that the three-body problem with forces other than Keplerian enters into this category, as the existence of attractive PODS seems to imply. A detailed numerical investigation of potential of (13) is currently underway.

We have shown that in the potential well of a $n > 2$ DOF Hamiltonian, there may exist under symmetry constraints new kinds of codim-1 invariant manifolds. While the actual interpretation of the potential presented is unimportant, the properties of HIMs as well as those of NHIMs are related to actual dynamics [20–22] and possibly to semi-classical analysis. Also, non-linear analysis, based on the same premises as the NHIM theory [13, 23] has to be pursued. Being large invariant manifolds, the stable and unstable manifolds of HIM and NHIM act at least locally as separatrices. Their stretching and folding may determine some of the fractal structure associated with high dimensional chaotic scattering.

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